Modeling the chemical space with (chemical) hypergraph

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Information about the chemical space gathered in Reaxy database can be used to test whether the chemical space has been growing randomly or not during the last 221 years. To do so, we compared the data with an Ërdos-Rényi (chemical) hypergraph model using some statistical measures in order to quantify the differences. In this talk, I will show (i) the main aspects of the Erdős–Rényi (chemical) hypergraph model we used to test the randomness of the chemical space growth and (ii) that the chemical space has been "moving away" from randomness at rate close to be an exponential rate.